FINANCIAL ASSISTANCE
FUNDING OPPORTUNITY ANNOUNCEMENT

U.S. Department of Energy

Office of Science
Office of Advanced Scientific Computing Research

Scientific Discovery Through Advanced Computing (SciDAC)

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APPLICATION DUE DATE: **March 6, 2006, 8:00 pm Eastern Time**

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NOTE: NEW REQUIREMENTS FOR GRANTS.GOV

Where to Submit: Applications must be submitted through Grants.gov to be considered for award.

Registration Requirements: There are several one-time actions you must complete in order to submit an application through Grants.gov (e.g., obtain a Dun and Bradstreet Data Universal Numbering System (DUNS) number, register with the Central Contract Registry (CCR), register with the credential provider, and register with Grants.gov). See www.grants.gov/GetStarted. Use the Grants.gov Organization Registration Checklist at www.grants.gov/assets/OrganizationRegCheck.doc to guide you through the process. Designating an E-Business Point of Contact (EBiz POC) and obtaining a special password called an MPIN are important steps in the CCR registration process. Applicants, who are not registered with CCR and Grants.gov, should allow at least 14 days to complete these requirements. It is suggested that the process be started as soon as possible.

Questions: Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. Part VII of this announcement explains how to submit other questions to the U.S. Department of Energy.

Application Receipt Notices

After an application is submitted, the Authorized Organization Representative (AOR) will receive a series of four e-mails. It is extremely important that the AOR watch for and save each of the emails. It may take up to two (2) business days from application submission to receipt of email Number 2. You will know that your application has reached DOE when the AOR receives email Number 4. You will need the Submission Receipt Number (email Number 1) to track a submission. The titles of the four e-mails are:

Number 1 - Grants.gov Submission Receipt Number
Number 2 - Grants.gov Submission Validation Receipt for Application Number
Number 3 - Grants.gov Grantor Agency Retrieval Receipt for Application Number
Number 4 - Grants.gov Agency Tracking Number Assignment for Application Number

After receipt of email Number 4, you can view your application at DOE's e-Center, http://e-center.doe.gov. A User Id and password are required. If you already have a User Id and password you do not need to re-register.

VERY IMPORTANT – Download PureEdge Viewer: In order to download the application package, you will need to install PureEdge Viewer. This small, free program will allow you to access, complete, and submit applications electronically and securely. For a free version of the software, visit the following web site: www.grants.gov/DownloadViewer.

TABLE OF CONTENTS

E. Evaluation and Administration by Non-Federal Personnel
F. Intellectual Property Developed under this Program
G. Notice of Right to Request Patent Waiver
H. Notice Regarding Eligible/Ineligible Activities
I. Reference Material

PART I – FUNDING OPPORTUNITY DESCRIPTION

SUMMARY: The Office of Science (SC) and the National Nuclear Security Administration (NNSA), U.S. Department of Energy (DOE), hereby announce interest in receiving applications for projects in the Scientific Discovery through Advanced Computing (SciDAC) research program. (Note: NSF will participate in the following Science Applications – Climate Modeling and Simulation and High Energy and Nuclear Physics with Petabytes.) The SciDAC program was initiated in 2001 as a partnership involving all SC program offices—Advanced Scientific Computing Research, Basic Energy Sciences, Biological and Environmental Research, Fusion Energy Sciences, High-Energy Physics and Nuclear Physics—to fully realize the potential of emerging petascale computers at that time for advancing scientific discovery. Researchers have achieved key scientific insights in a number of areas of National importance, yet many challenges of multi-scale, multi-disciplinary problems now facing science programs in DOE require advanced modeling and simulation capabilities on petascale computers. A second challenge is driven by the need for capture, storage, transmission, sharing and analysis of large-scale experimental and observational data, as well as data from simulations. This Notice is seeking applications that contribute to:

- The creation of a comprehensive, scientific computing software infrastructure that fully integrates applied mathematics, computer science, and computational science in the physical, biological, and environmental sciences for scientific discovery at the petascale level, and
- A new generation of data management and knowledge discovery tools for the large data sets obtained from large experimental facilities and from high end simulations.

Applications are sought that:

- Address obtaining significant insight into, or actually solve, a challenging problem of National scientific or engineering significance clearly related to DOE missions through computational science,
- Create scientific simulation codes that: achieve high single node performance; scale to thousands of nodes and tens-of-thousands of processors; and can be readily ported to other computer architectures,
- Develop applied mathematics and computer science methodology focused on computational science at the petascale and work with application teams to apply innovations,
- Integrate computational science with discipline-driven applications through teaming and partnerships with computer scientists and applied mathematicians,
- Engage experimental and observational data-intensive science, and/or
- Empower new scientific communities to achieve scientific discovery through computational science.

Prospective applicants should observe that the program is structured to be interdisciplinary and multi-institutional in nature. The Department's National Nuclear Security Administration is a partner in this program.

SUPPLEMENTARY INFORMATION:

Background:

1. Scientific Discovery through Advanced Computing

Advanced scientific computing will be a key contributor to scientific research in the 21st Century. Within the Office of Science (SC), scientific computing programs and facilities are already essential to progress in many areas of research critical to the Nation. Major scientific challenges exist in all SC research programs that can best be addressed through advances in scientific supercomputing, e.g., designing materials with selected properties, elucidating the structure and function of proteins, understanding and controlling plasma turbulence, and designing new particle accelerators. To help ensure its missions are met, SC is bringing together advanced scientific computing and scientific research in an integrated program entitled "Scientific Discovery Through Advanced Computing."

The Opportunity and the Challenge

During the past five years, the SciDAC program has clearly shown the benefits of teaming computational scientists, computer scientists and applied mathematicians in tackling challenging scientific problems. It has demonstrated that important scientific accomplishments are possible through simulation and modeling with focused collaboration and active partnership of domain scientists, applied mathematicians, and computer scientists. Successes have been documented in such areas as accelerator design, chemistry, combustion, climate modeling, and fusion. The program has also demonstrated that large scale simulation offers some of the most cost-effective opportunities for answering a number of scientific questions in areas, such as the fundamental structure of matter and the production of heavy elements in supernovae.

Extraordinary advances in computing technology in the past decade have set the stage for a major advance in scientific computing. . Within the next five to ten years, computers 1,000 times faster than today's terascale computers will become available. These advances herald a new era in scientific computing. In FY 2004 DOE's Office of Science launched an aggressive program to develop and deploy leadership-class computing facilities and announced a twenty-year scientific facilities roadmap that will provide a rich scientific infrastructure for the next two decades. A copy of the plan may be found at:
http://www.sc.doe.gov/Sub/Facilities_for_future/20-Year-Outlook-screen.pdf.

To exploit this opportunity, these computing advances must be translated into corresponding increases in the productivity of the scientific codes used to model physical, chemical, and biological systems. *This is a daunting problem.* Current advances in computing and networking technologies are being driven by market forces in the commercial sector, not by scientific computing. Harnessing commercial computing technology for scientific research poses problems unlike those encountered in previous supercomputers, in magnitude, as well as in kind. A comparable challenge applies to harnessing commercial network technology for the integration of scientific applications through networks to achieve required end-to-end performance. Towards

the end of this decade new systems are expected to emerge which will offer new architectures for scientific computation. New advances in mathematics, algorithms, computer science, and an ever-changing array of new computer architectures make the field of computational science one of continuing challenges.

The Investment Plan of the Office of Science

To take advantage of the opportunity offered by petascale computers, SC will fund a set of coordinated investments as outlined in its long-range plan for scientific computing, *Scientific Discovery through Advanced Computing,* (See Footnote Number 1[1]) submitted to Congress on March 30, 2000. First, it will create a *Scientific Computing Software Infrastructure* that bridges the gap between the advanced computing technologies being developed by the computer industry and the scientific research programs sponsored by the Office of Science. Specifically, SC plans to:

- Create a new generation of *Scientific Simulation Codes* that take full advantage of the extraordinary computing capabilities of terascale computers.
- Create the *Mathematical and Computing Systems Software* to enable the Scientific Simulation Codes to effectively and efficiently use terascale computers.
- Create a *Distributed Science Software Environment* to enable management, dissemination, and analysis of large data sets from simulation-intensive and experimental/observational-intensive science.

These activities are supported by a *Scientific Computing Hardware Infrastructure* that will evolve to meet the needs of its research programs. The *Hardware Infrastructure* provides the stable computing resources needed by the scientific applications; responds to innovative advances in computer technology that impact scientific computing; and allows the most appropriate and economical resources to be used to solve each class of problems. Specifically, SC plans to support:

- A *Flagship Computing Facility,* the National Energy Research Scientific Computing Center (NERSC), to provide robust, high-end computing resources needed by a broad range of scientific research programs.
- *Leadership Computing Facilities*, at Oak Ridge National Laboratory to provide very large scale computing resources tailored for specific scientific applications.
- *Capability resources* to support code development, scalability testing and other development activities to prepare application codes for terascale and petascale computations.
- *Early access to new emerging systems architectures,* e.g., BlueGene/L, to port and tune codes that may benefit from such systems.

These systems will evolve over the course of the next five years into petascale systems with hundreds of thousands of processors representing a variety of computer architectures to meet the needs of the SciDAC computational applications, as well as other computational science needs of the Office of Science.

The allocation of computing resources available to individual projects will be not be part of this solicitation but will be contingent on review and award through the process as described at: http://hpc.science.doe.gov Within the available computational resources, every effort will be made to ensure that successful applications will have the resources needed to support their efforts.

The systems that are part of the *Hardware Infrastructure* are embedded in a networking environment for science, the Energy Sciences Network (ESnet), that delivers the end-to-end capabilities needed to support scientific applications, and is evolving into a hybrid of packet switched services and high bandwidth circuit switched services, perhaps directly over wavelengths. It is anticipated that some applications may need to negotiate services across multiple, independent networks to achieve end-to-end performance.

The Benefits

The *Scientific Computing Software Infrastructure,* along with the upgrades to the hardware infrastructure, will enable laboratory and university researchers to solve the most challenging scientific problems faced by the Office of Science at a level of accuracy and detail never before achieved. These developments will have significant benefit to all of the government agencies who rely on high-performance scientific computing to achieve their mission goals, as well as to the U.S. high-performance computing industry.

Request for Cooperative Agreement Applications

This notice requests applications for cooperative agreements in the Science Application areas discussed in Section 2 and in the Enabling Technologies areas discussed in Section 3, with the exception of sub-sections specifically requesting grant applications. Cooperative Agreements differ from grants in that there is continuing substantial involvement by DOE in the conduct of the research.

Successful applicants of Science Applications must devise a multi-disciplinary research strategy that addresses both the domain science and computational science challenges facing their simulation or data management issue.

Successful applicants of Enabling Technologies must ensure that source code is fully and freely available for use and modification throughout the scientific computing community via a preapproved open source process.

To ensure that the SciDAC program meets the broadest needs of the research community, the successful applications are expected to participate in the annual SciDAC meeting, develop and maintain a project web site, and interact with other program participants on cross-cutting issues. It is anticipated that up to approximately $36,000,000 will be available for grants and cooperative agreement awards in FY 2006. The DOE is under no obligation to pay for any costs associated with the preparation or submission of an application. DOE reserves the right to fund, in whole or in part, any, all, or none of the applications submitted in response to this Notice.

The following two sections are offered to provide background in-depth information on areas that are of interest to the Office of Science along with NNSA and NSF for: 1*) the scientific and technical applications for a number of science domains of importance to the DOE mission, and 2) the enabling technology dimensions needed to achieve the SciDAC vision.*

2. Science Applications

The SciDAC program is structured as a set of coordinated investments across all SC mission areas with the goal of achieving breakthrough scientific advances via computer simulation that are impossible using theoretical or laboratory studies alone. In addition, the use of advanced computing technologies to accelerate scientific discovery is not limited to simulation-based science. It can also be applied to improving experimental science. Over the five years of the SciDAC program, researchers have achieved key scientific insights in a number of areas of National importance, including fusion, combustion, climate modeling, high energy and nuclear physics, and astrophysics. These advances have been accomplished through the development of state-of-the-art-simulation codes. The results of these simulations, together with associated theory and experiment, help ensure that the U.S. maintains a leadership role in science and technology.

The major source of acceleration in simulation-based science has been the strength and depth of partnerships among application domains, computer science, and applied mathematics. *Applications for research in the scientific domains must include a plan for partnerships that integrate advanced applied mathematics and computer science technologies with the proposed domain-specific efforts.* In addition, the plan may request additional resources for closely related computer science and applied mathematics research to ensure adequate integration. Work proposed in computer science or applied mathematics should be clearly identified. Additional information on the approach for partnerships is outlined in Section 3.

Challenges and opportunities remain in a number of scientific domains. Applications are sought for the following domains.

Accelerator Science and Simulation: A comprehensive, coherent petascale simulation capability for the U.S. particle and nuclear accelerator community is critical for the near and long-term priorities of DOE's Office of Science. High Energy Physics priorities are driven by optimization needs of existing HEP accelerators, such as the B-Factory and Tevatron, design of possible future accelerators, such as ILC other next-generation facilities, and maintaining a vital DOE accelerator R&D program. Near-term Nuclear Physics facility priorities are the Rare Isotope Accelerator (RIA) and the Continuous Electron Beam Accelerator Facility (CEBAF) Upgrade. In the longer term the Office of Nuclear Physics will explore the development of an electron-nucleus collider that would allow the gluon saturation of nuclear matter to be seen. Topic areas for modeling needs therefore include: high-accuracy computation of modes for superconducting RF cavities; realistic simulation of wakefield effects; parallelization of Radio Frequency Quadrapole (RFQ) simulations; self-consistent 3D calculations of Coherent Synchrotron Radiation; (CSR) forces and their effects on the beam; electron cooling of heavy-ion beams; optimization of Particle In Cell (PIC) codes; and adaptive mesh techniques for intense beams. Accelerator simulation codes which run on a variety of platforms, scale to petaflops and many thousands of processors, which are robust, documented, and can be easily

used by accelerator researchers at all DOE HEP and NP facilities, and are well integrated with visualization capacities will have the greatest impact on the field.
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Astrophysics: Computational astrophysics encompasses many research areas of interest and relevance to high-energy physics, nuclear physics, and Advanced Simulation and Computing. SciDAC applications for work in astrophysical and cosmological simulations are invited and will be judged in part based on their relevance to these program missions. While some examples of topical research areas are given below, successful SciDAC applications need not be limited to these areas.

Modeling of explosive astrophysical events, including Type Ia supernovae, gamma-ray bursts, X-ray bursts and core collapse supernovae is needed, not only for the quantitative understanding of the mechanics of supernovae, but also because all of these type of events produce unique nucleosynthesis products responsible for nearly all of the elements in the solar system and in living creatures. In addition, detailed simulations of these objects, in conjunction with astrophysical data, can shed new light on the physics of particle interactions and the properties of fundamental particles.

In particular, Type Ia supernovae are significant scientifically because of their use as standard candles in determining the expansion rate of the universe for measurements of dark energy, a technique which can be improved by a quantitative understanding of the transition from white dwarf stars to supernovae. Simulations of other types of supernovae and astrophysical objects also need to be performed to determine whether they can be used as standard candles, and what systematic variations limit their utility. A detailed simulation of core collapse supernovae brings together nuclear physics including neutrino physics, fluid dynamics, radiation transport of neutrinos, and general relativity and successful simulations could advance knowledge of nucleosynthesis and the properties of fundamental particles.

Unknown particles and forces (so-called dark matter and dark energy) make up 95% of the universe. DOE and NASA have both identified dark energy as a priority in their science programs. The two agencies have laid out a plan for a space-based, competed Joint Dark Energy Mission (JDEM) to determine the nature of dark energy. In addition, DOE supports several current experiments which are aimed at directly detecting cosmic dark matter or producing it in high-energy collisions. Computational techniques, which couple 2- and 3-dimensional simulations of complex astrophysical phenomena and structures with ground and space-based observations of dark matter and dark energy will be necessary to shed light on the properties of these unknown agents and perhaps interpret possible discoveries.

Other topics of interest include, but are not limited to: simulations of celestial objects, such as gamma ray bursts, to study the astrophysical acceleration mechanisms that produce the highest energy cosmic rays; simulations of dynamical processes which can explain and predict the

intergalactic magnetic fields which affect the propagation of these particles; cosmic microwave background (CMB) simulations required to understand the CMB data from the very early universe; and simulations, which can predict the imprint of gravitational waves on the CMB to directly see inflation in the early universe.

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Climate Modeling and Simulation: SciDAC climate modeling applications program continues to lead the evolution of DOE's long-standing climate modeling and simulation research agenda. The program, focused on developing, testing and applying climate simulation and prediction models that stay at the leading edge of scientific knowledge and computational technology, is tightly integrated with the goals of the Climate Change Prediction Program (CCPP; http://www.science.doe.gov/ober/CCRD/model.html) to advance climate change science and improve climate change projections using state-of-the-science coupled climate models, on time scales of decades to centuries and space scales of regional to global.
DOE is currently funding the testing, development, evaluation of high-end climate models and their use to answer strategic questions related to DOE's mission. Thus, the high priority areas: continued improvement in the representation of key processes in the current version of high-end climate models; continued development of frameworks that will test the above representations in the fully coupled system; and issues associated with running the fully coupled climate model efficiently on high-performance scientific supercomputers that are either available, or being envisaged under the Leadership Computing Facility at ORNL and other high-end computing resources available for DOE researchers.

The program will continue the development of climate models of the future based on theoretical foundations and improved computational methods that have the potential to run efficiently on current and future generations of high-performance scientific supercomputers. The intent is to increase dramatically both the accuracy and throughput of computer model-based predictions of future climate system response to the increased atmospheric concentrations of greenhouse gases. This notice requests applications in the following two areas:

1. Renewal applications for cooperative agreements for continued successful development of prototype climate models of the future including new formulations, numerical methods, algorithms and computational techniques, that will underpin the construction of production-quality coupled climate general circulation models in the next five-year time frame. The requests must clearly demonstrate progress under past support, e.g., model formulations that accurately simulate critical climate processes, efficient algorithms that execute on high-end computer architectures, such as multi-threaded and processor-in-memory designs. Renewal application requests should be roughly at previous level of funding or less. Multiple-year funding of awards is expected, with out-year funding contingent upon the availability of appropriated funds, progress of the research, and programmatic needs.

2. The DOE CCPP and NSF Climate and Large Scale Dynamics (CLD) programs are jointly sponsoring Small Grants for Exploratory Research (SGER) applications for exploratory research related to model development of the Community Climate System Model (CCSM). Information on the CCSM, including the CCSM Scientific Steering Committee may be found at: http://www.ccsm.ucar.edu/. These grants are intended for focused research on a particular aspect of CCSM that has received inadequate attention or that has been identified as a gap in understanding/simulation by the relevant CCSM working groups. SGER applications must include a statement about how the research proposed will benefit near-term, high priority CCSM development, being as explicit as possible about the issue(s) that will be addressed by the intended research.

   Examples of near-term high priorities are: improving tropical variability simulations including El Niño Southern Oscillation (ENSO); improving the representation of the Arctic Ocean hydrological cycle; testing of aerosol-cloud parameterizations to address the indirect effect of aerosols; and incorporation of terrestrial carbon cycle processes. The research should be designed to ultimately lead to testing of parameterization schemes for potential inclusion in the next version of the CCSM. The request should not exceed $25,000 and the duration is typically 12-18 months. Larger requests will be considered provided there is strong justification. Contingent on availability of funds, a maximum of 10 awards will be made.
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Computational Biology: GTL encompasses many types of data, each with algorithm research and development challenges in analyzing data for a broad range of purposes. Examples of objectives include:

- New generation of high-throughput, automated, annotation pipeline tools that keep pace with the exponentially increasing output of current and next-generation sequencing technologies. These tools should conform to current accuracy requirements and be compatible with existing downstream proteomic, expression and systems data formats.
  - New algorithms with improved comparative approaches to annotate organism and community sequences, identifying, for example, promoter and ribosome-binding sites, repressor and activator sites, and operon and regulon sequences.
  - Protein-function inference from sequence homology, fold type, protein interactions, and expression.
  - Automated linkage of gene, protein, and function catalog to phylogenetic, regulatory, structural, and metabolic relationships.

- Identify peptides, proteins, and their post-translational modifications of target proteins in mass spectrometry (MS) data.
  - New MS identification algorithms for tandem MS.

- Quantitate changes in cluster expression data from arrays or MS.
    - New expression data-analysis algorithms.
- Automatically identify interacting protein events in fluorescence resonance energy transfer (FRET) confocal microscopy.
    - New automated processing of images and video to interpret protein localization in the cell and to achieve high-throughput analysis.
- Reconstruct protein machines from 3D cryoelectron microscopy.
    - New automated multi-image convolution and reconstruction algorithms.
- Compare metabolite levels under different cell conditions.
    - Algorithms for metabolite method analysis, both global and with spatial resolution.

Modeling complex biological systems will require new methods to treat the vastly disparate length and time scales of individual molecules, molecular complexes, metabolic and signaling pathways, functional subsystems, individual cells, and, ultimately, interacting organisms and ecosystems. Such systems act on time scales ranging from microseconds to thousands of years. The systems must couple to huge databases created by an ever-increasing number of high-throughput experiments. Challenges include determining the right calculus to describe regulation, metabolism, protein interaction networks, and signaling in a way that allows quantitative prediction. Possible solutions include use of differential equations, stochastic or deterministic methods, control theory or ad hoc mathematical network solutions, binary or discrete value networks, Chaos theory, and emerging and future new abstractions.

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Fusion Science: Improved simulation and modeling of fusion systems is essential for achieving the predictive scientific understanding needed to make fusion energy practical. The success of the ITER project strongly depends on the development of such validated predictive capability. Current large scale simulations in fusion plasma science include integrated modeling of electromagnetic wave interactions with plasmas described in the MHD approximation as well as work on understanding the plasma edge. Efforts are also underway in modeling plasma turbulence and macroscopic stability using two-fluid or extended MHD models.

Integrated simulation of magnetic fusion systems involves the simultaneous modeling of the core and edge plasma regions, as well as the interaction of the plasma with material surfaces. In each of these plasma regions, there is transport of heat, particles and momentum driven by plasma turbulence, abrupt rearrangements of the plasma caused by large-scale instabilities, and interactions with neutral atoms and electromagnetic waves. Many of these processes must be computed on short time and spatial scales, while the predictions of integrated modeling are needed for the entire device on longer time scales. This mix of physical complexity and widely

differing spatial and temporal scales in integrated modeling, results in a unique computational challenge.

In addition, the further development of collaborative technologies is critical to the success of the Fusion Energy Sciences program. Such fusion collaboratories will be essential to fully exploit present and future facilities, especially since the international fusion community is moving toward fewer and larger machines, such as ITER, and large scale integrated simulations.

Applications to be funded under this announcement should focus on:

- Efforts to further develop and facilitate international fusion collaboratories since international cooperation is of increasing importance for Fusion Energy Sciences.
- The development of an integrated software environment for multi-physics, multi-scale simulations of fusion systems, including the algorithms, software methodology, and framework for designing, building, and validating the software components needed for comprehensive plasma simulations.

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Groundwater Reactive Transport Modeling and Simulation: Scientifically rigorous models of subsurface reactive transport that accurately simulate contaminant mobility across multiple length scales remain elusive. The Department of Energy has long-term clean-up and management responsibility for its Cold War era production facilities, and the responsibility for monitoring the behavior of contaminants in ground waters around existing and future waste disposal and storage areas. Conceptual model development and computer simulation of contaminant transport are important elements of the decision-making process for environmental remediation and monitoring. Innovative, new approaches to performing multi-physics, multi-phase, multi-component, multi-dimensional subsurface reactive flow and transport simulations that take advantage of high performance, "leadership class" computing capabilities are sought. Specific areas of potential interest include:

- Computational methods exploring efficient means of solving very large systems of equations, inherent in subsurface reactive transport modeling, on high performance computers.
- Incorporation of methods of model abstraction, parameter sensitivity and uncertainty analyses into high performance computer simulations of subsurface reactive transport.
- Incorporation of characterization data from field measurement techniques such as seismic geophysical analyses or, at a smaller scale, high resolution laboratory measurement techniques into computational models.
- Methods exploring optimal hardware architecture and, optimal conceptual and computational model complexity for subsurface reactive transport simulation.
- Computational methods examining the scalability ("upscaling"), spatial variability and temporal variability of biogeochemical reactions occurring at the molecular level to the field scale.
- Development of parallel programming and output visualization tools enabling subsurface scientists to more easily access and utilize the high performance computing assets within DOE.

Simulation of subsurface reactive transport processes on high performance, "leadership class" computers has not been widely utilized by subsurface scientists or environmental managers responsible for remediation decision-making. The intent of this call is to explore what options "leadership class" computing can bring to the understanding of subsurface reactive transport of fluids and contaminants and to foster collaborations among subsurface scientists and computational scientists in order to facilitate use of these high performance computing assets for environmental applications.

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High-Energy Physics: SciDAC supports cross-disciplinary research into cutting-edge problems in scientific computing. As pioneers in the computing sciences since their inception, HEP researchers are fully committed to continuing to advance the state of the art of scientific computing and applying the most modern techniques and tools to our work.

The HEP mission has three research thrusts The Energy Frontier (i.e., testing and refining our understanding of the standard model), The Dark Universe (i.e., investigating the nature of dark energy, dark matter, and the origins of the cosmos), and Neutrinos (i.e., measuring the properties and behavior of this unique family of particles). Each of these domains faces different computational and data management challenges, many of which are ideally suited to the SciDAC program of work.

To fully realize our scientific goals and make the most effective use of the large facilities and collaborations which characterize the current generation of HEP research, we will need simulation, data management, and data analysis and visualization applications which run on a wide variety of computer architectures, from commodity clusters to specialized machines to supercomputers and which are easily accessible to researchers at small universities, as well as large National Laboratories

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High Energy and Nuclear Physics with Petabytes: High energy physics and nuclear physics experiments stand at the threshold of revolutionary challenges and opportunities. Experiments at colliding beams and the next generation of fixed targets are key to the advancing the understanding of the physics or the universe on the smallest length and time scales, and at the level at which the fundamental particles transition into matter.

With the next generation of physics accelerators and detectors, instruments with an analog data rate of a petabyte a second will yield petabytes per year after data selection and compression. Even with this high degree of selectivity, revolutionary new approaches to data management and data analysis are needed to allow scientific intuition and intellect deal with the daunting volume of data. This notice seeks applications that address the data intensive research challenges of high

energy physics and nuclear physics, including the production environment for distributed data-intensive science, and provide innovative approaches to data analysis environments characterized by having tens to hundreds of scientists simultaneously accessing refined datasets of tens of terabytes.

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Materials Science & Chemistry: Materials science and chemistry remain key research areas for the National Nuclear Security Administration. Understanding and accurately modeling material properties, reactions, and interactions, and doing so on length scales that range in excess of 10 orders of magnitude, is integral to the program. This includes the development of improved simulation methods for complex quantum systems enabled by developing supercomputer technology. The Advanced Simulation and Computing (ASC) program is interested in research in this area that can be applied to the computer modeling of materials.

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Nuclear Physics: Increased computational resources, algorithmic development and a coherent petascale effort spanning all of nuclear structure and reactions are important for the advancement of nuclear physics, including nuclear astrophysics, neutrino physics and fundamental symmetries. Nuclear structure and reactions play an essential role in the science to be investigated at the Rare Isotope Accelerator (RIA) and in nuclear physics applications to the Science-Based Stockpile Stewardship (SBSS) program and other DOE mission needs, such as energy research and threat reduction. Future theory progress on the equation of state of the quark-gluon plasma and the evaluation of the dynamics of the reaction observed at the Relativistic Heavy Ion Collider (RHIC) can be advanced through significant increase of the computational and algorithmic development needed to solve relativistic radiative transport and covariant second order dissipative hydrodynamics equations on this terascale level.

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Quantum Chromodynamics (QCD): The goal of the SciDAC program in QCD is to create opportunities for major scientific advances through highly accurate simulations of the lattice gauge theory. The physics issues to be addressed include calculations of matrix elements needed for precise tests of the standard model, determination of the properties of strongly interacting matter under extreme conditions of temperature and density, the internal structure of nucleons and other strongly interacting particles, and QCD calculations of hard-to-measure baryon-baryon interactions needed for low energy nuclear and hypernuclear physics. Major improvements in lattice calculations will be driven by improvements in computer hardware, software environments, algorithms, and theoretical formulations of QCD. As well, the regular structure of lattice calculations has made them amenable to efficient execution on specially designed computers whose design echoes that regularity. The enormous amount of computation needed to achieve meaningful physics results has made the cost effectiveness of such computers a necessity.

A major accomplishment of the SciDAC 1 QCD program was the development of a unified programming environment that has enabled the U.S. lattice gauge community to achieve high efficiency on a wide variety of terascale computers. The platform exploits the special features of QCD calculations which made them particularly well suited to massively parallel computers. This interface now underpins QCD calculations on MPP machines, such as Seaborg at NERSC, specialized machines such as the QCDOC at BNL, and the commodity clusters being built at FNAL and JLab. The software infrastructure includes tools to archive and retrieve files annotated with XML metadata consistent with the newly created International Lattice Data Grid.

There are many possible directions for further progress. One immediate need, to advance these important calculations in High Energy and Nuclear Physics, is adapting the current simulation environment to additional hardware architectures, such as cluster computers based on multi-core chips or the IBM Blue Gene/L. Another is enhancing the simulation environment both to execute the best existing codes with higher performance and to facilitate the rapid development and evaluation of new algorithms and methods.

The data sets generated by realistic lattice simulations are large enough so that new software tools are needed to manage them and access to them to ensure that their physics potential is most effectively exploited. As well, new tools are needed to visualize the increasingly complex data analyses being applied to the results of these calculations.

HEP POC: Craig Tull, (301)-903-0468 Craig.Tull@science.doe.gov
NP POC: Sidney A. Coon, (301)-903-7878 Sidney.A.Coon@science.doe.gov

Radiation Transport: Determining the processes and interactions of radiation transport is an extremely complex proposition. To date we have been limited both in our scientific understanding and our computational resources. Without the compute power to move beyond diffusion methods to Monte Carlo or discrete ordinate multi-particle, multi-group transport methods, those using as few approximations as possible, we cannot fully investigate transport, or resulting energy deposition, of radiation.

In weapons, as in other complex systems, such as engines and reactors, transport is a key element of the coupled, multi-physics present. The development of models and codes capable of realistically dealing with radiation in 2 and 3D is critical to the predictive capability of the codes and therefore the confidence we place in the computational results upon which decisions are based.

The Advanced Simulation and Computing (ASC) program and the Office of Science are interested in research in this area that can be applied to the computer modeling of transport.

NNSA POC: Dr. Njema Frazier, 202-586-5789 Njema.Frazier@nnsa.doe.gov
NP POC: Sidney A. Coon, (301)-903-7878 Sidney.A.Coon@science.doe.gov

Turbulence: The development of models and codes that can incorporate the exact equations governing the Reynolds stresses, and which predict dynamic instabilities are still sought. Presently, Large Eddy Simulation (LES) methods, viscosity modeling methods, and fluid approximation model methods stand at the forefront of our ability to model turbulent flow. However, the physics of turbulence, and the mathematical and computational representation of

that physics are still open research areas that require ongoing effort. The Advanced Simulation and Computing (ASC) program is interested in research in this area that can be applied to the computer modeling of turbulence.

NNSA POC: Dr. Njema Frazier, 202-586-5789 Njema.Frazier@nnsa.doe.gov

3. Enabling Computational Technologies

The key to the success of the SciDAC program has been the power of multidisciplinary teams that bring together experts in the scientific discipline, computer science, and applied mathematics. Multidisciplinary teams have achieved progress that could not have been made in any other way. It is increasingly hard for a small team of experts in a single area to develop a state-of-the-art simulation code that uses the latest mathematical algorithms and runs effectively on today's complex computer architectures. Successes to-date have relied on new infrastructure in applied mathematics, computer science, and distributed computing technology.
This program element has several dimensions. It must provide the following:

- Comprehensive, integrated, scalable, and robust high performance computing software infrastructure to enable effective use of leadership class computing resources.
- Comprehensive, integrated, scalable, and robust distributed computing technologies for experimental facilities and science.
- Targeted efforts to integrate advanced applied mathematics and computer science technologies into selected applications projects.

All applications must include a plan for supporting their software over the long term. All applications must also include a plan for developing partnerships with science applications.

The framework for accomplishing these objectives includes, but is not limited to, Centers for Enabling Technologies (CET), Science Institutes, and Partnerships. Centers for Enabling Technologies are large teams centered around developing software infrastructure with a specific focus, such as performance analysis or advanced tools for differential equations. SciDAC Institutes are university-led and are complementary to the CETs, addressing additional dimensions as discussed below. For example, there could be an Institute centered around large scale optimization for engineering problems. Finally, Partnerships provide support to integrate computational science with discipline-driven applications. Applications to this notice can request funding for any one of these three elements, however, requests for Partnerships must be included with requests for support under science domain topics.

Centers for Enabling Technologies: Centers for Enabling Technologies (CET) address the Mathematical and Computing Systems Software Environment element of the SciDAC Scientific Computing Software Infrastructure. This infrastructure envisions a comprehensive, integrated, scalable, and robust high performance software environment, which overcomes difficult technical challenges to enable the effective use of terascale and petascale systems by SciDAC applications. CETs address needs for: new algorithms which scale to parallel systems having hundreds-of-thousands of processors; methodology for achieving portability and interoperability

of complex high performance scientific software packages; operating systems and runtime tools and support for application execution performance and system management; and effective tools for feature identification, data management and visualization of petabyte-scale scientific data sets.

CETs also address the Distributed Science Software Environment element of the SciDAC Scientific Computing Software Infrastructure. This infrastructure recognizes the use of advanced computing technologies to improve experimental science, as well as accelerate scientific discovery through modeling and simulation. This can be accomplished through the development and application of advanced data and analysis capabilities, computation in support of experiment, and technologies for the automation of experiments.

CETs provide the essential computing and communications infrastructure for support of SciDAC applications. The CET effort encompasses a multi-discipline approach with activities in:

- Algorithms, methods, and libraries -- Algorithms, methods and libraries that are fully scalable to many thousands of processors with full performance portability.
- Program development environments and tools -- Component-based, fully integrated, terascale and petascale program development and tools, which scale effectively and provide maximum utility and ease-of-use to developers and scientific end users.
- Operating system and runtime software and tools -- Systems software that scales to hundreds-of-thousands of processors, supports high performance application-level communication, I/O, performance analysis and optimization, and provides the highest levels of fault tolerance, reliability, manageability, and ease of use for end users, tool developers and system administrators.
- Visualization and data management systems -- Scalable, intuitive systems fully supportive of SciDAC application requirements for moving, storing, analyzing, querying, manipulating and visualizing multi-petabytes of scientific data and objects.
- Distributed data management and computing tools – Scalable and secure systems for the analysis of large volumes of data produced at experimental facilities, often through complex workflows, and consumed by a large and distributed user community, as well as end-to-end network tools and services to support high-end applications.
- Real-time computing at experimental facilities

The complexity of these challenges and the strong emphasis on scalability, interoperability and portability requires novel approaches in the proposed technical research and the research management structure. CETs emphasize working directly with applications and the support of application partnerships to enable:

- Development and application of mathematical and/or computing systems software that allows scientific simulation codes to take full advantage of the extraordinary capabilities of terascale and petascale computers.
- Close working relationships with application teams and other SciDAC teams to ensure that the most critical computer science and applied mathematics issues are addressed in a timely and comprehensive fashion.

- Addressing all aspects of the successful research software lifecycle including transition of a research code into a robust production code and long term software evolution and maintenance and end user support. *The software lifecycle must be addressed in all CET applications.*

In order to foster broad availability and use of CET-developed code, all CET applications must specify the type of open source license that will be used and the mechanisms, including web sites, workshops, and other community-based activities that will be used to disseminate information about CET software.

SciDAC Institutes: Science and engineering are critically dependent on the existence of robust and reliable high-performance computing applications codes. These application codes are in turn critically dependent on the algorithms and software developed by the high-performance computer science community. The SciDAC Institutes are university-led centers of excellence intended to complement the efforts of the Centers for Enabling Technologies, as well as centers formed under-specific science domains. This will be achieved by focusing on major software issues through a range of collaborative research interactions. Applications are sought on software methods or techniques that are important to a number of specific science problems.

Characteristics of a SciDAC Institute are that it may:

- Concentrate efforts to develop, test, maintain, and support optimal algorithms, programming environments, systems software and tools, and applications software.
- Focus on a single general method or technique(for example, large scale optimization for engineering problems).
- Be a focal point for bringing together a critical mass of leading experts from multiple disciplines to focus on key problems in a particular area of enabling technologies.
- Forge relationships between experts in software development, scientific application domains, high performance computing, and industrial partners (e.g., a "Computational End Station" allowing computational scientists to improve and utilize community codes where coordination around integrated modeling strategies, algorithms and specialized suites of software tools is important for success).
- Reach out to engage a broader community of scientists in the activities of scientific discovery through advanced computation and collaboration.
- Have a dimension of training and outreach in high performance computing topics, including for graduate students and postdocs.
- Scientific applications that sufficiently integrate the above will be considered for award.

Applications may include scope to ensure that SciDAC tools are robust and widely available on diverse platforms through building and supporting test environments, coordination of software releases, and implementation of mechanisms to facilitate porting and tuning.

Applications should describe the organizational model which might be: 1) part of a university, 2) a separate organization, like a non-profit corporation, or 3) a university-led distributed center involving multiple institutions, that may include other universities, industry, non-profit organizations, Federal Laboratories and Federally Funded Research and Development Centers (FFRDCs), which include the DOE National Laboratories.

Partnerships: The major source of progress in simulation-based science depends upon the strength and depth of partnerships among application domains, computer science, and applied mathematics. Scientific Application Partnerships offer support for this type of multidisciplinary interaction.

Science Application Partnerships (SAP or Partnerships) are a broad activity of the Office of Advanced Scientific Computing Research (ASCR) formed when applied mathematics and computer science research can significantly enhance a targeted science area of importance to SC. Funding for these Partnerships is shared between ASCR and the other SC offices along with oversight responsibilities. Thus SAP projects must have components relevant to each office that is involved. This SciDAC program element seeks to fund activities that form a partnership between computational mathematics and computer science with a science domain.

Thus applications submitted under Section 2. Science Applications may identify specific, targeted activities to be considered for funding as Scientific Application Partnerships. The SAP projects are to be managed by a single lead PI and Institution and should identify the other Investigators as "Application Science (S)", "Applied Mathematics (M)" or "Computer Science (CS)". It is envisioned that SAP projects will demonstrate a balance between S and M/CS personnel.

The key elements and characteristics expected for science applications projects are:

- Focus on a targeted application science area that lies within the scope of topics listed in Section 2 under Science Applications.
- Leverage for inserting existing or new applied mathematics and computer science research into an identified science area to enable or otherwise significantly enhance the field. It may provide the insertion of new technologies directly into application codes or explore new programming and/or modeling methodology for petascale applications.
- It may involve collocation of computational mathematicians and computer scientists with application teams. These individuals may also act as liaisons to foster interactions with CETs.
- A cohesive project with a shared goal. Each institution and investigator must clearly identify their contribution towards this goal. Projects that appear disjoint in this regard are discouraged.

Potential partnership activities should be clearly identified in a Science Application submission, and the requested funding for partnership efforts in computer science and applied mathematics should be included with the other project costs on the Budget Page. However, applications should also provide the requested computer science and applied mathematics costs separately in an appendix in order to be considered for support by the Office of Advanced Scientific Computing Research under a partnership agreement.

ASCR POCs: Anil Deane (301) 903-1465 deane@mics.doe.gov; Thomas Ndousse (301) 903-9960 tndousse@er.doe.gov; Fred Johnson (301) 903-3601 fjohnson@er.doe.gov; Gary Johnson (301) 903-4361 garyj@er.doe.gov; Mary Anne Scott (301) 903-6368 scott@er.doe.gov; Yukiko Sekine (301) 903-5997 yukiko.sekine@science.doe.gov

PART II – AWARD INFORMATION

A. TYPE OF AWARD INSTRUMENT.

DOE anticipates awarding grants and cooperative agreements under this program announcement. If it is determined that a cooperative agreement is the appropriate award instrument, the nature of the Federal involvement will be included in a special award condition.

B. ESTIMATED FUNDING.

It is anticipated that in Fiscal Year 2006 SciDAC partners will have up to approximately $36,000,000 available to support new SciDAC projects. The number of awards will be determined by the number of excellent applications and the total funds available for this program, and subject to the availability of funds. These funds provided by participating offices may be up to the following: ASCR, $25,000,000; BER, $2,250,000; FES, $1,000,000; NNSA, $4,000,000; NP; $1,000,000; and HEP, $2,000,000

C. MAXIMUM AND MINIMUM AWARD SIZE.

Ceiling (i.e., the maximum amount for an individual award made under this announcement): N/A

Floor (i.e., the minimum amount for an individual award made under this announcement): N/A

D. EXPECTED NUMBER OF AWARDS.

The number of awards will be contingent on satisfactory peer review, the availability of appropriated funds and the size of the awards.

E. ANTICIPATED AWARD SIZE.

N/A

F. PERIOD OF PERFORMANCE.

N/A

G. TYPE OF APPLICATION.

N/A

PART III - ELIGIBILITY INFORMATION

A. ELIGIBLE APPLICANTS.

DOE Eligibility Criteria: Any university or other institution of higher education or other non-profit or for-profit organization, non-Federal agency or entity, is eligible for a grant or cooperative agreement. An unaffiliated individual also is eligible for a grant or cooperative agreement. Researchers from Federally Funded Research and Development Centers (FFRDCs) or DOE National Laboratories should respond to Program Announcement LAB 06-04.

A companion Program Announcement to DOE Laboratories will be posted on the Office of Science Grants and Contracts web site at http://www.science.doe.gov/grants/.

B. COST SHARING

Cost sharing is not required.

C. OTHER ELIGIBILITY REQUIREMENTS.

N/A

PART IV – APPLICATION AND SUBMISSION INFORMATION

A. ADDRESS TO REQUEST APPLICATION PACKAGE.

Application forms and instructions are available at Grants.gov. To access these materials, go to http://www.grants.gov, select "Apply for Grants", and then select "Download Application Package". Enter the CFDA and/or the funding opportunity number located on the cover of this announcement and then follow the prompts to download the application package. NOTE: You will not be able to download the Application Package unless you have installed PureEdge Viewer (See: http://www.grants.gov/DownloadViewer).

B. LETTER OF INTENT AND PRE-APPLICATION.

1. Letter of Intent.

Letters of Intent are due January 23, 2006, 4:30 pm Eastern Time.

Potential applicants are required to submit a one (1) to two (2) page Letter of Intent by January 23, 2006, which includes the title of the proposed effort, the program area addressed, the names of the principal investigator and all senior personnel, participating institutions, organizational approach, projected funding request (if possible) and summary/abstract. For multi-institution applications, a single Letter of Intent should be submitted by the PI of the lead institution. Letters of Intent will be reviewed for conformance with the guidelines presented in this Notice and suitability in the technical areas specified in this Notice. A response to the Letters of Intent encouraging or discouraging formal applications will be communicated to the applicants by January 30, 2006.

Letters-of-Intent should be submitted electronically as an email attachment (not pdf) to scidac-2@mics.doe.gov. Please use the phrase "SciDAC Science Application-PI_Lastname-Insitution" or "SciDAC Enabling Technology-PI_Lastname-Institution" in the subject line (where PI Lastname is the surname of the lead PI and Institution is the lead institution). A copy to the appropriate POC is also encouraged.

2. Pre-application.

Pre-applications are not required.

C. CONTENT AND FORM OF APPLICATION – SF 424 (R&R)

You must complete the mandatory forms and any applicable optional forms (e.g., SF-LLL-Disclosure of Lobbying Activities) in accordance with the instructions on the forms and the additional instructions below**. Files that are attached to the forms must be in Adobe Portable Document Format (PDF) unless otherwise specified in this announcement.**

1. **SF 424 (R&R)**
   Complete this form first to populate data in other forms. Complete all the required fields in accordance with the pop-up instructions on the form. To activate the instructions, turn on the "Help Mode" (Icon with the pointer and question mark at the top of the form). The list of certifications and assurances referenced in Field 18 can be found on the Applicant and Recipient Page at http://grants.pr.doe.gov.

2. **RESEARCH AND RELATED Other Project Information.**
   Complete questions 1 through 5 and attach files. The files must comply with the following instructions:

   Project Summary/Abstract (Field 6 on the Form)
   The project summary/abstract must contain a summary of the proposed activity suitable for dissemination to the publication. It should be a self-contained document that identifies the name of the applicant, the project director/principal investigator(s), the project title, the objectives of the project, a description of the project, including methods to be employed, the potential impact of the project (i.e., benefits, outcomes), and major participants (for collaborative projects). This document must not include any proprietary or sensitive business information as the Department may make it available to the public. The project summary must not exceed 1 page when printed using standard 8.5" by 11" paper with 1" margins (top, bottom, left and right) with font not smaller than 11 point. To attach a Project Summary/Abstract, click "Add Attachment."

   Project Narrative (Field 7 on the form)

   The narrative comprises the research plan for the project and must be 20 pages or less, including tables and figures, but excluding forms and certifications, when printed using standard 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) and font not smaller than 11 point. EVALUATORS WILL ONLY REVIEW THE NUMBER OF PAGES SPECIFIED IN THE PRECEDING SENTENCE. Letters of commitment for collaboration of non-funded collaborators and short curriculum vitae of all senior personnel must be included in the application. Applications not meeting these requirements will be deemed ineligible during the initial screening process. The major part of the narrative should be devoted to a description and justification of the proposed project, including details of the methods to be used. It should also include a timeline for the major activities of the proposed project, and should indicate which project personnel will be responsible for which activities. Do not include any Internet addresses (URLs) that provide information necessary to review the application, because the information contained in these sites will not be reviewed. See Part VIII.D for instructions on how to mark proprietary application information. To attach a Project Narrative, click "Add Attachment."

   The first page of your narrative must include the following information:

   Applicant/Institution:
   Street Address/City/State/Zip:

Principal Investigator:
Address:
Telephone Number:
Email:
DOE/Office of Science Program Office:
DOE/Office of Science Program Office Technical Contact:
DOE Grant Number (if Renewal or Supplemental Application):
Is this a Collaboration? If yes, please list ALL Collaborating Institutions/PIs***** and indicate which ones will also be submitting applications.

**** Note that collaborating applications must be submitted separately.***

The project narrative must include:

- Project Objectives.
  This section should provide a clear, concise statement of the specific objectives/aims of the proposed project.

- Merit Review Criterion Discussion.
  The section should be formatted to address each of the merit review criterion and sub-criterion listed in Section V. A. Provide sufficient information so that reviewers will be able to evaluate the application in accordance with these merit review criteria. DOE WILL EVALUATE AND CONSIDER ONLY THOSE APPLICATIONS THAT ADDRESS SEPARATELY EACH OF THE MERIT REVIEW CRITERION AND SUB-CRITERION.

- Evaluation Phase
  This section must include a plan and metrics to be used to assess the success of the project.

- Project Performance Site
  Indicate the primary site where the work will be performed. If a portion of the work will be performed at any other sites, identify those sites, also.

- Biographical Sketch Appendix
  Provide a biographical sketch for the project director/principal investigator (PD/PI) and each senior/key person listed in Section A on the R&R Budget form. Provide the biographical sketch information as an appendix to your project narrative. Do not attach a separate file. The biographical sketch appendix will not count in the project narrative page limitation. The biographical information for each person must not exceed 2 pages when printed on 8.5" by 11" paper with 1 inch margins (top, bottom, left, and right) with font not smaller than 11 point and must include:

  Education and Training. Undergraduate, graduate and postdoctoral training, provide institution, major/area, degree and year.

  Research and Professional Experience: Beginning with the current position list,

in chronological order, professional/academic positions with a brief description.

Publications. Provide a list of up to 10 publications most closely related to the proposed project. For each publication, identify the names of all authors (in the same sequence in which they appear in the publication), the article title, book or journal title, volume number, page numbers, year of publication, and website address if available electronically.

Patents, copyrights and software systems developed may be provided in addition to or substituted for publications.

Synergistic Activities. List no more than 5 professional and scholarly activities related to the effort proposed.

- *Current and Pending Support*. List all current and pending support. For each organization providing support, show the total award amount for the entire award period (including indirect costs) and the number of person-months per year to be devoted to the project. Concurrent submission of an application to other organizations for simultaneous consideration will not prejudice its review.

- *Identification of Potential Conflicts of Interest or Bias in Selection of Reviewers.* Provide the following information in this section:

  Collaborators and Co-editors: List in alphabetical order all persons, including their current organizational affiliation, who are, or who have been, collaborators or co-authors with you on a research project, book or book article, report, abstract, or paper during the 48 months preceding the submission of this application. Also, list any individuals who are currently, or have been, co-editors with you on a special issue of a journal, compendium, or conference proceedings during the 24 months preceding the submission of this application. If there are no collaborators or co-editors to report, state "None."

  Graduate and Postdoctoral Advisors and Advisees: List the names and current organizational affiliations of your graduate advisor(s) and principal postdoctoral sponsor(s) during the last 5 years. Also, list the names and current organizational affiliations of your graduate students and postdoctoral associates during the past 5 years.

Bibliography & References Cited (Field 8 on the form)
Provide a bibliography of any references cited in the Project Narrative. Each

reference must include the names of all authors (in the same sequence in which they appear in the publication), the article and journal title, book title, volume number, page numbers, and year of publication. Include only bibliographic citations. Applicants should be especially careful to follow scholarly practices in providing citations for source materials relied upon when preparing any section of the application. In order to reduce the number of files attached to your application, please provide the Bibliography and References Cited information as an appendix to your project narrative. Do not attach a file in field 8. This appendix will not count in the project narrative page limitation.

Facilities & Other Resources (Field 9 on the form) This information is used to assess the capability of the organizational resources, including subawardee resources, available to perform the effort proposed. Identify the facilities to be used (Laboratory, Animal, Computer, Office, Clinical and Other). If appropriate, indicate their capacities, pertinent capabilities, relative proximity, and extent of availability to the project. Describe only those resources that are directly applicable to the proposed work. Describe other resources available to the project (e.g., machine shop, electronic shop) and the extent to which they would be available to the project. In order to reduce the number of files attached to your application, please provide the Facility and Other Resource information as an appendix to your project narrative. Do not attach a file in field 9. This appendix will not count in the project narrative page limitation.

Equipment (Field 10 on the form)
List major items of equipment already available for this project and, if appropriate identify location and pertinent capabilities. In order to reduce the number of files attached to your application, please provide the Equipment information as an appendix to your project narrative. Do not attach a file in field 10. This appendix will not count in the project narrative page limitation.

Other Attachment (Field 11 on the form)
If you need to elaborate on your responses to questions 1-5 on the "Other Project Information" document, provide the information as an appendix to your project narrative. Do not attach a file in field 11.

Also, attach the following files:
No additional files are required.

3. RESEARCH AND RELATED BUDGET.
Complete the Research and Related Budget form in accordance with the instructions on the form (Activate Help Mode to see instructions) and the following instructions. You must complete a separate budget for each year of support requested. The form will generate a cumulative budget for the total project period. You must complete all the mandatory information on the form before the NEXT PERIOD button is activated. You may request funds under any of the categories listed as long as the item and amount are necessary to perform the proposed work, meet all the criteria for allowability under the applicable Federal cost principles, and are not prohibited by the funding restrictions in

this announcement (See PART IV, G).

Budget Justification (Field K on the form).
Provide the required supporting information for the following costs (See R&R Budget instructions): equipment; domestic and foreign travel; participant/trainees; material and supplies; publication; consultant services; ADP/computer services; subaward/consortium/contractual; equipment or facility rental/user fees; alterations and renovations; and indirect cost type. Provide any other information you wish to submit to justify your budget request. If cost sharing is required, provide an explanation of the source, nature, amount and availability of any proposed cost sharing. Attach a single budget justification file for the entire project period in Field K. The file automatically carries over to each budget year.

4. **RESEARCH AND RELATED BUDGET.**

Budgets for Subawardees, other than DOE FFRDC Contractors. You must provide a separate cumulative R&R budget for each subawardee that is expected to perform work estimated to be more than $100,000 or 50 percent of the total work effort (whichever is less). If you are selected for award, you must submit a multi-year budget for each of these subawardee (See Section IV.D for submission of Subawardees' multi-year budgets). Download the R&R Budget Attachment from the R&R SUBAWARD BUDGET ATTACHMENT(S) FORM and e-mail it to each subawardee that is required to submit a separate budget. Note: Subwardees must have installed PureEdge Viewer before they can complete the form. After the Subawardee has e-mailed its completed budget back to you, attach it to one of the blocks provided on the form. Use up to 10 letters of the subawardee's name (plus .xfd) as the file name (e.g., ucla.xfd or energyres.xfd).

5. **SF-LLL Disclosure of Lobbying Activities** If applicable, complete SF- LLL. Applicability: If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the grant/cooperative agreement, you must complete and submit Standard Form - LLL, "Disclosure Form to Report Lobbying."

D. SUBMISSIONS FROM SUCCESSFUL APPLICANTS.
The Department anticipates that no additional submissions will be required. However, it reserves the right to request additional or clarifying information for any reason deemed necessary.

E. SUBMISSION DATES AND TIMES.

1. Letter of Intent Due Date. Potential applicants are required to submit a one (1) to two (2) page Letter-of-Intent by January 23, 2006, which includes the title of the proposed effort, the program area addressed, the names of the principal investigator and all senior personnel, participating institutions, organizational approach, projected funding request (if possible) and summary/abstract. For multi-institution applications, a single Letter-of-Intent should be submitted by the PI of the lead institution. Letters of Intent will be reviewed for conformance

with the guidelines presented in this Notice and suitability in the technical areas specified in this Notice. A response to the Letters of Intent encouraging or discouraging formal applications will be communicated to the applicants by January 30, 2006.

Letters-of-Intent should be submitted electronically as an email attachment (not pdf) to: scidac-2@mics.doe.gov. Please use the phrase "SciDAC Science Application-PI_Lastname-Insitution" or "SciDAC Enabling Technology-PI_Lastname-Institution" in the subject line (where PI Lastname is the surname of the lead PI and Institution is the lead institution). A copy to the appropriate POC is also encouraged.

2. Application Due Date. Formal applications in response to this Notice submitted to the Office of Science must be submitted electronically through Grants.Gov by **March 6, 2006, 8:00 pm Eastern Time** to be considered for award. In addition, a copy of the full application should also be submitted electronically as a single pdf file to scidac-2@mics.doe.gov. The email should use the phrase "SciDAC Science Application" or "SciDAC Enabling Technology," as appropriate, in the subject line. APPLICATIONS RECEIVED AFTER THE DEADLINE WILL NOT BE REVIEWED OR CONSIDERED FOR AWARD.

F. GOVERNMENTAL REVIEW

This program is subject to Executive Order 12372 (Intergovernmental Review of Federal Programs) and the regulations at 10 CFR Part 1005.

One of the objectives of the Executive order is to foster an intergovernmental partnership and a strengthened federalism. The Executive order relies on processes developed by State and local governments for coordination and review of proposed Federal financial assistance.

Applicants should contact the appropriate State Single Point of Contact (SPOC) to find out about, and to comply with, the State's process under Executive Order 12372. The names and addresses of the SPOCs are listed on the Web site of the Office of Management and Budget at http://www.whitehouse.gov/omb/grants/spoc.html.

H. FUNDING RESTRICTIONS.

Cost Principles**.** Costs must be allowable in accordance with the applicable Federal cost principles referenced in 10 CFR Part 600.

Pre-award Costs**.** Recipients may charge to an award resulting from this announcement pre-award costs that were incurred within the ninety (90) calendar day period immediately preceding the effective date of the award, if the costs are allowable in accordance with the applicable Federal cost principles referenced in 10 CFR Part 600. Recipients must obtain the prior approval of the contracting officer for any pre-award costs that are for periods greater than this 90 day calendar period.

Pre-award costs are incurred at the applicant's risk. DOE is under no obligation to reimburse such costs if for any reason the applicant does not receive an award or if the award is made for a lesser amount than the applicant expected.

H. OTHER SUBMISSION AND REGISTRATION REQUIREMENTS

1. Where to Submit.

APPLICATIONS MUST BE SUBMITTED THROUGH GRANTS.GOV TO BE CONSIDERED FOR AWARD. Submit electronic applications through the "Apply for Grants" function at www.Grants.gov. If you have problems completing the registration process or submitting your application, call Grants.gov at 1-800-518-4726 or send an email to support@grants.gov.

2. Registration Process.

You must COMPLETE the one-time registration process (all steps) before you can submit your first application through Grants.gov (See www.grants.gov/GetStarted). **We recommend that you start this process at least two weeks before the application due date**. It may take 14 days or more to complete the entire process. Use the Grants.gov Organizational Registration Checklists at http://www.grants.gov/assets/OrganizationRegCheck.doc to guide you through the process. IMPORTANT: During the CCR registration process, you will be asked to designate an E-Business Point of Contact (EBIZ POC). The EBIZ POC must obtain a special password called "Marketing Partner identification Number" (MPIN).

Part V - APPLICATION REVIEW INFORMATION

A. CRITERIA

1. Initial Review Criteria.
Prior to a comprehensive merit evaluation, DOE will perform an initial review in accordance with 10 CFR 605.10(b).

2. Merit Review Criteria. Applications will be subjected to scientific merit review (peer review) and will be evaluated against the following evaluation criteria which are listed in descending order of importance codified at 10 CFR 605.10(d):

1. Scientific and/or Technical Merit of the Project;
2. Appropriateness of the Proposed Method or Approach;
3. Competency of Applicant's Personnel and Adequacy of Proposed Resources; and
4. Reasonableness and Appropriateness of the Proposed Budget.

In considering item 1 particular attention will be paid to:

a) The potential of the proposed project to make a major scientific advance in a specific domain or to have a significant impact in the effectiveness of SciDAC applications researchers;
b) The demonstrated capabilities of the applicants to perform basic research and transform these research results into software that can be widely deployed;
c) Knowledge of and coupling to previous efforts in scientific simulation;
d) For enabling technology applications, the likelihood that the algorithms, methods, mathematical libraries, and software components that result from this effort will have impact on or is extensible to science disciplines outside of the SciDAC applications projects;
e) Identification and approach to software integration and long term support issues, including component technology, documentation, test cases, tutorials, end user training, and quality maintenance and evolution; and
f) Extent to which the application incorporates broad community (industry/academia/other federal programs) interaction;

In considering item 2, particular attention will be paid to

a) Quality of the plan for effective coupling to emerging advances in enabling technology or to applications researchers;
b) Quality and clarity of the proposed work schedule and deliverables;
c) Quality of the proposed approach to intellectual property management and open source licensing;
d) Quality of the plan for effective collaboration among participants; and

e) Quality of the plan for ensuring communication with other advanced computation and simulation efforts or enabling technology efforts.

The evaluation will include program policy factors, such as the relevance of the proposed research to the terms of the announcement and the agency's programmatic needs.

External peer reviewers are selected with regard to both their scientific expertise and the absence of conflict-of-interest issues. Non-federal reviewers will often be used, and submission of an application constitutes agreement that this is acceptable to the investigator(s) and the submitting institution. Reviewers will be selected to represent expertise in the science and technology areas proposed, applications groups that are potential users of the technology, and related programs in other Federal Agencies or parts of DOE.

B. REVIEW AND SELECTION PROCESS.

1. Merit Review.

Applications will be subjected to formal merit review (peer review) and will be evaluated against the evaluation criteria codified at 10 CFR 605.10(d) listed above, as well as the additional criteria listed above.

2. Selection.

The Selection Official will consider the merit review recommendation, program policy factors, and the amount of funds available.

3. Discussions and Award.

The Government may enter into discussions with a selected applicant for any reason deemed necessary, including but not limited to: (1) the budget is not appropriate or reasonable for the requirement; (2) only a portion of the application is selected for award; (3) the Government needs additional information to determine that the recipient is capable of complying with the requirements in 10 CFR part 600 and 605; and/or (4) special terms and conditions are required. Failure to resolve satisfactorily the issues identified by the Government will preclude award to the applicant.

C. ANTICIPATED NOTICE OF SELECTION AND AWARD DATES.

DOE is striving to make awards within eight months. The time interval begins on the date applications are due or the date the application is received, if there is no specified due date/deadline.

Part VI - AWARD ADMINISTRATION INFORMATION

A. AWARD NOTICES.

1. Notice of Selection.
DOE will notify applicants selected for award. This notice of selection is not an authorization to begin performance. (See Part IV.G with respect to the allowability of pre-award costs.)

Organizations whose applications have not been selected will be advised as promptly as possible. This notice will explain why the application was not selected.

2. Notice of Award.
A Notice of Financial Assistance Award issued by the contracting officer is the authorizing award document. It normally includes, either as an attachment or by reference: 1. Special Terms and Conditions; 2. Applicable program regulations, if any; 3. Application as approved by DOE; 4. DOE assistance regulations at 10 CFR part 600, or, for Federal Demonstration Partnership (FDP) institutions, the FDP terms and conditions; 5. National Policy Assurances to Be Incorporated As Award Terms; 6. Budget Summary; and 7. Federal Assistance Reporting Checklist, which identifies the reporting requirements.

B. ADMINISTRATIVE AND NATIONAL POLICY REQUIREMENTS.

1. Administrative Requirements.

The administrative requirements for DOE grants and cooperative agreements are contained in 10 CFR Part 600 and 10 CFR Part 605 (See: http://ecfr.gpoaccess.gov), except for grants made to Federal Demonstration Partnership (FDP) institutions. The FDP terms and conditions and DOE FDP agency specific terms and conditions are located on the National Science Foundation web site at http://www.nsf.gov/awards/managing/fed_dem_part.jsp.

2. Special Terms and Conditions and National Policy Requirements.

Special Terms and Conditions and National Policy Requirements.
The DOE Special Terms and Conditions for Use in Most Grants and Cooperative Agreements are located at http://grants.pr.doe.gov. The National Policy Assurances To Be Incorporated As Award Terms are located at http://grants.pr.doe.gov.

Intellectual Property Provisions.
The standard DOE financial assistance intellectual property provisions applicable to the various types of recipients are located at http://www.gc.doe.gov/techtrans/sipp_matrix.html.

C. REPORTING.
Reporting requirements are identified on the Federal Assistance Reporting Checklist, DOE F4600.2, attached to the award agreement.

PART VII - QUESTIONS/AGENCY CONTACTS

A. QUESTIONS

Questions regarding the content of the announcement must be submitted through the "Submit Question" feature of the DOE Industry Interactive Procurement System (IIPS) at http://e-center.doe.gov. Locate the program announcement on IIPS and then click on the "Submit Question" button. Enter required information. You will receive an electronic notification that your question has been answered. DOE will try to respond to a question within 3 business days, unless a similar question and answer have already been posted on the website.

Questions relating to the registration process, system requirements, how an application form works, or the submittal process must be directed to Grants.gov at 1-800-518-4726 or support@grants.gov. DOE cannot answer these questions.

Questions regarding the program (**technical**) requirements should be directed to:

Agency Contacts:

Walt Polansky, Mary Anne Scott, or Dave Goodwin, Office of Advanced Scientific Computing Research, Telephone (301) 903-5800; ascr-scidac_coordination@mics.doe.gov

PART VIII - OTHER INFORMATION

A. MODIFICATIONS.

Notices of any modifications to this announcement will be posted on Grants.gov and the DOE Industry Interactive Procurement System (IIPS). You can receive an email when a modification or an announcement message is posted by joining the mailing list for this announcement through the link in IIPS. When you download the application at Grants.gov, you can also register to receive notifications of changes through Grants.gov.

B. GOVERNMENT RIGHT TO REJECT OR NEGOTIATE.

DOE reserves the right, without qualification, to reject any or all applications received in response to this announcement and to select any application, in whole or in part, as a basis for negotiation and/or award.

C. COMMITMENT OF PUBLIC FUNDS.

The Contracting Officer is the only individual who can make awards or commit the Government to the expenditure of public funds. A commitment by other than the Contracting Officer, either explicit or implied, is invalid.

D. PROPRIETARY APPLICATION INFORMATION.

Patentable ideas, trade secrets, proprietary or confidentional commercial or financial information, disclosure of which may harm the applicant, should be included in an application only when such information is necessary to convey an understanding of the proposed project. The use and disclosure of such data may be restricted, provided the applicant includes the following legend on the first page of the project narrative and specifies the pages of the application which are to be restricted:

"The data contained in pages _____ of this application have been submitted in confidence and contain trade secrets or proprietary information, and such data shall be used or disclosed only for evaluation purposes, provided that if this applicant receives an award as a result of or in connection with the submission of this application, DOE shall have the right to use or disclose the data herein to the extent provided in the award. This restriction does not limit the government's right to use or disclose data obtained without restriction from any source, including the applicant."

To protect such data, each line or paragraph on the pages containing such data must be specifically identified and marked with a legend similar to the following:

"The following contains proprietary information that (name of applicant) requests not be released to persons outside the Government, except for purposes of review and evaluation."

E. EVALUATION AND ADMINISTRATION BY NON-FEDERAL PERSONNEL.

In conducting the merit review evaluation, the Government may seek the advice of qualified non-Federal personnel as reviewers. The Government may also use non-Federal personnel to

conduct routine, nondiscretionary administrative activities. The applicant, by submitting its application, consents to the use of non-Federal reviewers/administrators. Non-Federal reviewers must sign conflict of interest and non-disclosure agreements prior to reviewing an application. on-Federal personnel conducting administrative activities must sign a non-disclosure agreement.

F. INTELLECTUAL PROPERTY DEVELOPED UNDER THIS PROGRAM.

Patent Rights. The government will have certain statutory rights in an invention that is conceived or first actually reduced to practice under a DOE award. 42 U.S.C. 5908 provides that title to such inventions vests in the United States, except where 35 U.S.C. 202 provides otherwise for nonprofit organizations or small business firms. However, the Secretary of Energy may waive all or any part of the rights of the United States subject to certain conditions. (See "Notice of Right to Request Patent Waiver" in paragraph G below.)

Rights in Technical Data. Normally, the government has unlimited rights in technical data created under a DOE agreement. Delivery or third party licensing of proprietary software or data developed solely at private expense will not normally be required except as specifically negotiated in a particular agreement to satisfy DOE's own needs or to insure the commercialization of technology developed under a DOE agreement.

G. NOTICE OF RIGHT TO REQUEST PATENT WAIVER.

Applicants may request a waiver of all or any part of the rights of the United States in inventions conceived or first actually reduced to practice in performance of an agreement as a result of this announcement, in advance of or within 30 days after the effective date of the award. Even if such advance waiver is not requested or the request is denied, the recipient will have a continuing right under the award to request a waiver of the rights of the United States in identified inventions, i.e., individual inventions conceived or first actually reduced to practice in performance of the award. Any patent waiver that may be granted is subject to certain terms and conditions in 10 CFR 784.

Domestic small businesses and domestic nonprofit organizations will receive the patent rights clause at 37 CFR 401.14, i.e., the implementation of the Bayh-Dole Act. This clause permits domestic small business and domestic nonprofit organizations to retain title to subject inventions. Therefore, small businesses and nonprofit organizations do not need to request a waiver.

H. N/A

I. N/A